Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:59 pm BST

PDB ID	:	5N98
Title	:	Crystal Structure of Drosophila DHX36 helicase in complex with TAGGGTTTT
Authors	:	Chen, W.-F.; Rety, S.; Guo, H.-L.; Wu, W.-Q.; Liu, N.-N.; Liu, Q.-W.; Dai, Y.-X.; Xi, X.-G.
Deposited on	:	2017-02-24
Resolution	:	2.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

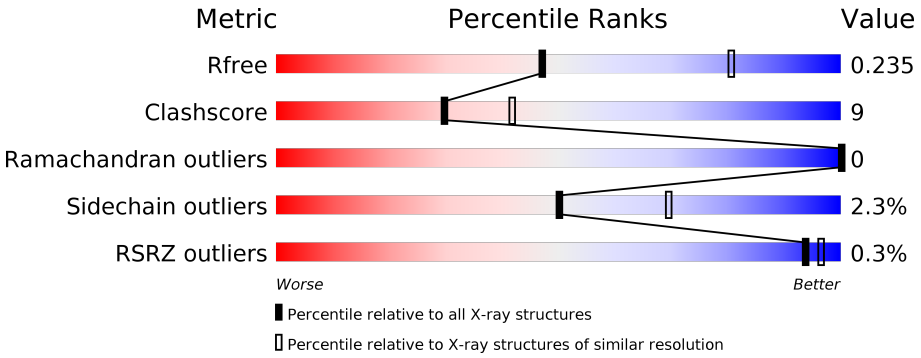
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	944	71% 18% • 10%
1	B	944	68% 21% • 10%
2	C	9	78% 22%
2	D	9	78% 11% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14157 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CG9323, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	849	Total	C	N	O	S	0	0	0
			6814	4304	1200	1265	45			
1	B	851	Total	C	N	O	S	0	0	0
			6829	4312	1202	1270	45			

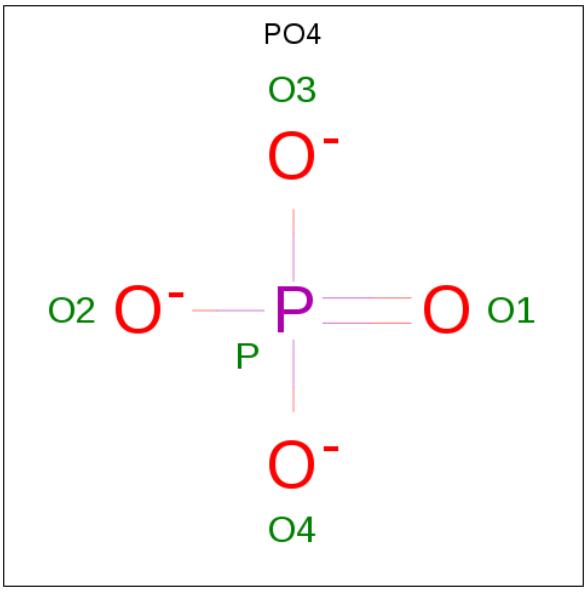
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	943	VAL	-	expression tag	UNP Q8SWT2
A	944	ASP	-	expression tag	UNP Q8SWT2
B	943	VAL	-	expression tag	UNP Q8SWT2
B	944	ASP	-	expression tag	UNP Q8SWT2

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*GP*GP*GP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			187	90	30	58	9			
2	D	9	Total	C	N	O	P	0	0	0
			187	90	30	58	9			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

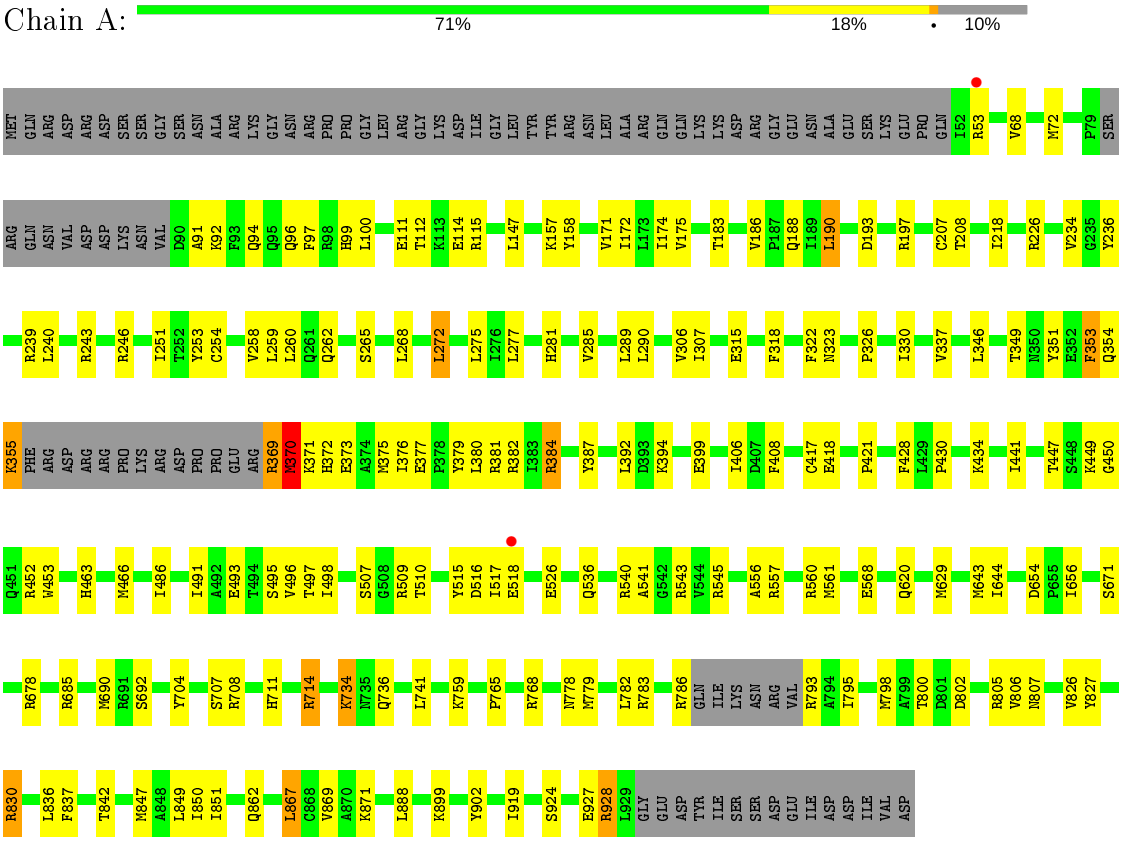
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	66	Total O 66 66	0	0
4	B	64	Total O 64 64	0	0
4	C	4	Total O 4 4	0	0
4	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

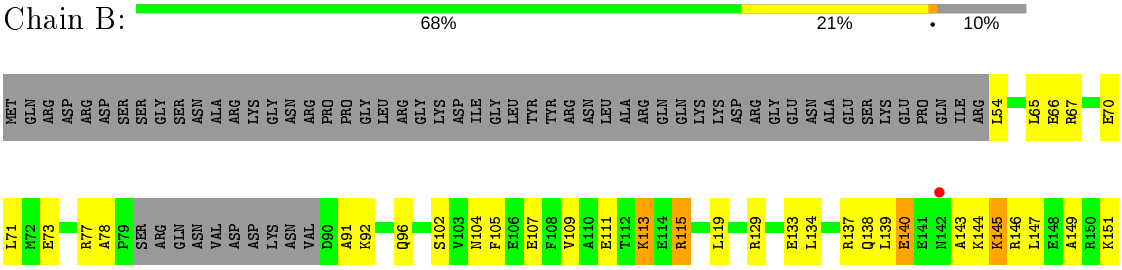
- Molecule 1: CG9323, isoform A

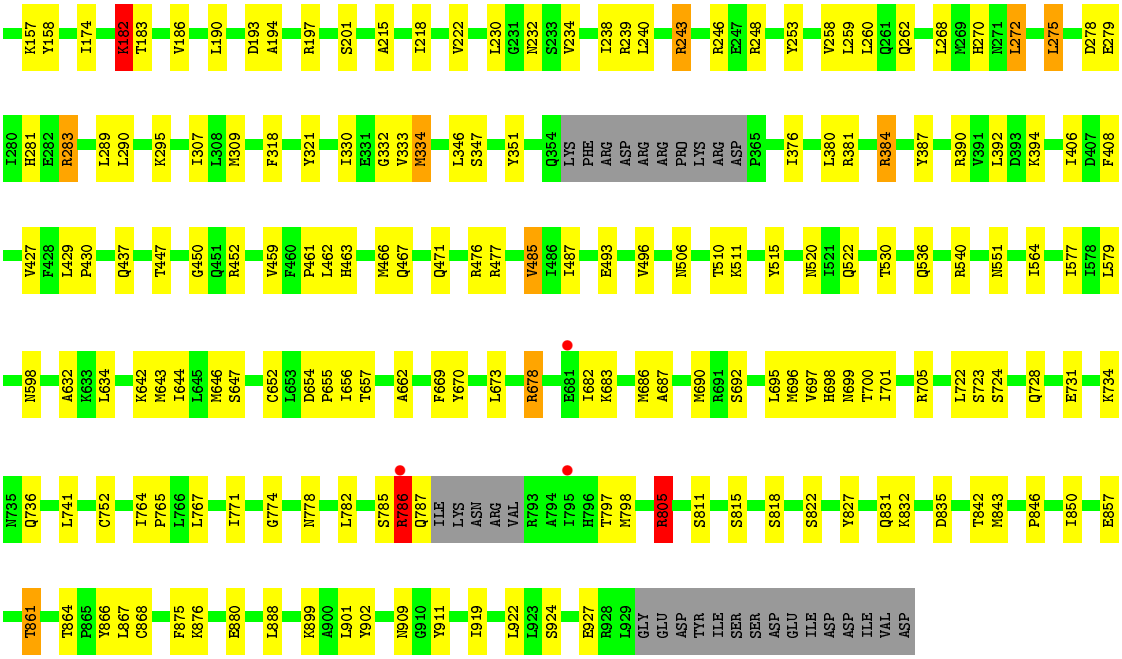
Chain A:



- Molecule 1: CG9323, isoform A

Chain B:





- Molecule 2: DNA (5'-D(P*TP*AP*GP*GP*GP*TP*TP*TP*T)-3')

Chain C:

- Molecule 2: DNA (5'-D(P*TP*AP*GP*GP*GP*TP*TP*TP*T)-3')

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	303.41Å 51.62Å 164.97Å 90.00° 114.43° 90.00°	Depositor
Resolution (Å)	56.84 – 2.76 138.12 – 2.76	Depositor EDS
% Data completeness (in resolution range)	92.5 (56.84-2.76) 92.5 (138.12-2.76)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.77Å)	Xtriage
Refinement program	PHENIX (dev_2427: ???)	Depositor
R, R_{free}	0.175 , 0.236 0.174 , 0.235	Depositor DCC
R_{free} test set	2828 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14157	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.49	0/6933	0.81	17/9353 (0.2%)
1	B	0.53	3/6950 (0.0%)	0.89	24/9378 (0.3%)
2	C	1.11	0/208	1.19	0/320
2	D	1.10	1/208 (0.5%)	1.16	0/320
All	All	0.54	4/14299 (0.0%)	0.87	41/19371 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	634	LEU	C-N	-7.50	1.20	1.34
1	B	678	ARG	CG-CD	-5.88	1.37	1.51
2	D	9	DT	C1'-N1	5.12	1.55	1.49
1	B	182	LYS	CB-CG	5.06	1.66	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	805	ARG	CG-CD-NE	-17.72	74.59	111.80
1	B	805	ARG	NE-CZ-NH1	15.99	128.29	120.30
1	B	678	ARG	CA-CB-CG	-13.95	82.71	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	545	ARG	CB-CG-CD	-13.82	75.66	111.60
1	B	805	ARG	NE-CZ-NH2	-13.64	113.48	120.30
1	B	805	ARG	CB-CG-CD	12.07	142.98	111.60
1	A	157	LYS	CA-CB-CG	-10.20	90.96	113.40
1	B	786	ARG	CB-CG-CD	-9.34	87.32	111.60
1	A	323	ASN	N-CA-CB	-9.33	93.80	110.60
1	A	714	ARG	CA-CB-CG	8.64	132.41	113.40
1	A	714	ARG	CB-CA-C	8.57	127.54	110.40
1	A	545	ARG	CG-CD-NE	8.42	129.49	111.80
1	B	334	MET	N-CA-C	-8.42	88.27	111.00
1	A	384	ARG	CG-CD-NE	-7.93	95.15	111.80
1	B	384	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	A	370	MET	C-N-CA	7.29	139.94	121.70
1	A	714	ARG	CB-CG-CD	6.52	128.56	111.60
1	B	786	ARG	CG-CD-NE	6.52	125.49	111.80
1	A	928	ARG	N-CA-CB	6.46	122.22	110.60
1	B	140	GLU	CA-CB-CG	6.27	127.20	113.40
1	A	545	ARG	CA-CB-CG	6.24	127.12	113.40
1	B	805	ARG	CD-NE-CZ	6.20	132.28	123.60
1	A	620	GLN	CA-CB-CG	6.06	126.74	113.40
1	B	283	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	A	384	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	137	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	B	332	GLY	C-N-CA	5.47	135.37	121.70
1	B	785	SER	C-N-CA	-5.47	108.03	121.70
1	B	678	ARG	CB-CG-CD	5.46	125.80	111.60
1	A	928	ARG	CA-CB-CG	5.45	125.38	113.40
1	B	786	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	384	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	A	190	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	B	182	LYS	CD-CE-NZ	5.26	123.80	111.70
1	B	115	ARG	CB-CG-CD	-5.26	97.93	111.60
1	A	289	LEU	CB-CG-CD2	-5.22	102.13	111.00
1	A	370	MET	CA-CB-CG	5.21	122.16	113.30
1	B	113	LYS	CD-CE-NZ	-5.17	99.81	111.70
1	B	722	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	B	115	ARG	CB-CA-C	-5.13	100.14	110.40
1	B	786	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	322	PHE	Peptide
1	A	353	PHE	Peptide
1	A	370	MET	Peptide
1	A	421	PRO	Peptide
1	A	862	GLN	Peptide
1	B	144	LYS	Peptide
1	B	805	ARG	Sidechain
1	B	861	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6814	0	6913	114	0
1	B	6829	0	6917	148	0
2	C	187	0	105	3	0
2	D	187	0	105	2	0
3	B	5	0	0	0	0
4	A	66	0	0	9	0
4	B	64	0	0	2	0
4	C	4	0	0	1	0
4	D	1	0	0	0	0
All	All	14157	0	14040	263	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:PRO:HB2	1:B:466:MET:HE3	1.39	1.03
1:B:683:LYS:NZ	1:B:811:SER:O	2.10	0.84
1:A:239:ARG:HB2	2:C:9:DT:H3'	1.60	0.83
1:B:690:MET:CE	1:B:699:ASN:HD21	1.91	0.82
1:B:333:VAL:HG12	1:B:334:MET:H	1.45	0.82
1:B:798:MET:N	1:B:805:ARG:HH12	1.77	0.81
1:B:289:LEU:HD11	1:B:577:ILE:HD12	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:THR:HG23	1:A:450:GLY:H	1.44	0.80
1:A:871:LYS:NZ	4:A:1002:HOH:O	2.14	0.80
1:B:447:THR:HG23	1:B:450:GLY:H	1.44	0.80
1:B:798:MET:O	1:B:805:ARG:NH1	2.15	0.79
1:B:463:HIS:HB3	1:B:466:MET:HG3	1.64	0.77
1:B:259:LEU:HD23	1:B:290:LEU:HD11	1.65	0.77
1:B:786:ARG:HG3	1:B:787:GLN:N	2.00	0.77
1:B:901:LEU:CD2	1:B:902:TYR:CZ	2.69	0.76
1:A:315:GLU:OE1	4:A:1001:HOH:O	2.04	0.74
1:B:515:TYR:OH	1:B:520:ASN:ND2	2.21	0.74
1:A:793:ARG:N	4:A:1003:HOH:O	2.21	0.73
1:A:370:MET:HA	1:A:372:HIS:H	1.54	0.72
1:B:333:VAL:CG1	1:B:334:MET:H	2.03	0.72
1:B:73:GLU:HG3	1:B:77:ARG:HH21	1.54	0.72
1:A:515:TYR:HE2	1:A:517:ILE:HD12	1.54	0.72
1:A:654:ASP:OD2	1:A:734:LYS:NZ	2.22	0.72
1:B:901:LEU:HD22	1:B:902:TYR:CE1	2.25	0.71
1:B:522:GLN:HE21	1:B:831:GLN:HE21	1.36	0.71
1:B:151:LYS:O	1:B:157:LYS:HE2	1.89	0.71
1:B:901:LEU:CD2	1:B:902:TYR:CE1	2.73	0.70
1:B:467:GLN:HB2	1:B:670:TYR:CZ	2.27	0.70
1:A:800:THR:OG1	1:A:802:ASP:OD1	2.07	0.69
1:B:822:SER:H	1:B:843:MET:HE2	1.58	0.69
1:B:215:ALA:HB3	1:B:238:ILE:HD11	1.75	0.69
1:A:259:LEU:HD23	1:A:290:LEU:HD11	1.74	0.68
1:A:349:THR:HG23	1:A:351:TYR:H	1.58	0.68
1:A:805:ARG:NH1	4:A:1005:HOH:O	2.26	0.68
1:A:463:HIS:HB3	1:A:466:MET:HG3	1.76	0.67
1:A:759:LYS:NZ	4:A:1004:HOH:O	2.24	0.67
1:A:850:ILE:HD13	1:A:869:VAL:HB	1.77	0.67
1:A:175:VAL:HG11	1:A:315:GLU:HG2	1.76	0.66
1:A:92:LYS:O	1:A:96:GLN:HG3	1.95	0.66
1:A:644:ILE:HG22	1:A:741:LEU:HD21	1.79	0.65
1:B:888:LEU:HD21	1:B:919:ILE:HG12	1.78	0.65
1:B:678:ARG:HG2	1:B:678:ARG:O	1.96	0.65
1:B:222:VAL:HG13	1:B:234:VAL:HG11	1.77	0.65
1:A:112:THR:HG21	1:A:268:LEU:HD13	1.80	0.64
1:A:193:ASP:OD1	1:A:197:ARG:NH1	2.32	0.62
1:B:92:LYS:O	1:B:96:GLN:HG3	2.00	0.62
1:B:239:ARG:HB2	2:D:9:DT:H3'	1.82	0.61
1:A:285:VAL:HG23	1:A:568:GLU:CD	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TYR:O	1:A:394:LYS:HE3	2.01	0.61
1:A:91:ALA:HB2	1:A:902:TYR:HD1	1.65	0.60
1:B:193:ASP:OD2	1:B:197:ARG:NH1	2.33	0.60
1:B:506:ASN:HD22	1:B:551:ASN:HD22	1.49	0.60
1:B:406:ILE:HD13	1:B:437:GLN:HB3	1.82	0.60
1:B:107:GLU:O	1:B:111:GLU:HG3	2.02	0.59
1:B:240:LEU:HD21	1:B:736:GLN:HB2	1.85	0.59
1:A:516:ASP:OD2	1:A:518:GLU:HB2	2.03	0.58
1:A:765:PRO:HG2	1:A:927:GLU:HG2	1.86	0.58
1:B:406:ILE:CD1	1:B:437:GLN:HB3	2.34	0.58
1:B:427:VAL:HG22	1:B:487:ILE:HA	1.84	0.58
1:A:171:VAL:HG22	1:A:306:VAL:HG22	1.86	0.58
1:A:800:THR:HG23	1:A:806:VAL:HG11	1.86	0.58
1:B:201:SER:O	1:B:248:ARG:HD3	2.04	0.57
1:B:643:MET:HE3	1:B:774:GLY:HA3	1.87	0.57
1:B:687:ALA:HB2	1:B:696:MET:HG3	1.87	0.57
1:B:73:GLU:HG3	1:B:77:ARG:NH2	2.19	0.57
1:B:643:MET:HE1	1:B:771:ILE:HA	1.85	0.57
1:B:861:THR:O	1:B:864:THR:N	2.35	0.57
1:A:68:VAL:O	1:A:72:MET:HG3	2.06	0.56
1:A:783:ARG:NH2	4:A:1006:HOH:O	2.31	0.56
1:A:786:ARG:HB3	1:A:795:ILE:H	1.71	0.56
1:A:375:MET:HG3	1:A:560:ARG:HE	1.68	0.56
1:B:109:VAL:HG22	1:B:268:LEU:HD11	1.88	0.56
1:A:387:TYR:HB2	1:A:392:LEU:HD21	1.88	0.56
1:B:644:ILE:HG22	1:B:741:LEU:HD11	1.86	0.56
1:B:798:MET:H	1:B:805:ARG:HH12	1.49	0.56
1:B:690:MET:HE1	1:B:699:ASN:HD21	1.70	0.55
1:A:370:MET:HA	1:A:372:HIS:N	2.20	0.55
1:B:506:ASN:HD22	1:B:551:ASN:ND2	2.04	0.55
1:B:239:ARG:HG3	2:D:10:DT:OP1	2.05	0.55
1:B:283:ARG:NH2	1:B:598:ASN:OD1	2.23	0.55
1:B:705:ARG:HD3	1:B:731:GLU:OE1	2.06	0.54
1:B:183:THR:HG21	1:B:218:ILE:HD13	1.89	0.54
1:A:924:SER:O	1:A:927:GLU:HG3	2.08	0.54
1:B:381:ARG:O	1:B:384:ARG:HD2	2.09	0.53
1:A:353:PHE:O	1:A:354:GLN:HG2	2.09	0.53
1:A:557:ARG:HG3	1:A:561:MET:HE3	1.90	0.53
1:B:157:LYS:HD3	1:B:157:LYS:N	2.23	0.53
1:A:486:ILE:HD13	1:A:498:ILE:HD13	1.91	0.53
1:A:172:ILE:HG22	1:A:326:PRO:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ILE:O	1:B:222:VAL:HG12	2.08	0.53
1:A:91:ALA:HB2	1:A:902:TYR:CD1	2.44	0.53
1:B:493:GLU:HG2	1:B:536:GLN:CG	2.38	0.53
1:A:240:LEU:HD21	1:A:736:GLN:HB2	1.91	0.52
1:A:685:ARG:NH1	4:A:1010:HOH:O	2.40	0.52
1:B:295:LYS:HE3	1:B:321:TYR:CE2	2.44	0.52
1:B:654:ASP:OD1	1:B:734:LYS:NZ	2.42	0.52
1:A:779:MET:CE	1:A:849:LEU:HD13	2.40	0.52
1:A:786:ARG:HG2	1:A:795:ILE:HD12	1.91	0.52
1:B:459:VAL:HG22	1:B:485:VAL:HG13	1.92	0.52
1:A:418:GLU:HG2	1:A:453:TRP:HZ2	1.75	0.52
1:A:258:VAL:O	1:A:262:GLN:HG3	2.09	0.52
1:B:65:LEU:HD13	1:B:880:GLU:HG3	1.92	0.51
1:B:832:LYS:HA	1:B:835:ASP:O	2.10	0.51
1:A:373:GLU:HG2	1:A:377:GLU:HG3	1.90	0.51
1:A:376:ILE:O	1:A:380:LEU:HG	2.09	0.51
2:C:10:DT:OP2	4:C:101:HOH:O	2.19	0.51
1:B:493:GLU:HG2	1:B:536:GLN:HG3	1.91	0.51
1:B:143:ALA:HA	1:B:146:ARG:HB2	1.93	0.51
1:A:449:LYS:O	1:A:452:ARG:HB3	2.11	0.51
1:B:190:LEU:HD11	1:B:307:ILE:HD11	1.92	0.51
1:B:657:THR:OG1	4:B:1101:HOH:O	2.19	0.51
1:A:158:TYR:CD1	1:A:330:ILE:HD12	2.46	0.51
1:A:782:LEU:HD12	1:A:798:MET:HB2	1.92	0.50
1:B:138:GLN:O	1:B:139:LEU:HD23	2.11	0.50
1:B:669:PHE:CE1	1:B:696:MET:HE1	2.46	0.50
1:B:797:THR:HA	1:B:805:ARG:HH22	1.77	0.50
1:B:351:TYR:CE2	1:B:408:PHE:HB2	2.46	0.50
1:B:510:THR:HG22	1:B:511:LYS:N	2.26	0.50
1:B:662:ALA:HB2	1:B:697:VAL:HG11	1.93	0.50
1:A:315:GLU:N	1:A:315:GLU:OE1	2.43	0.50
1:B:692:SER:OG	1:B:695:LEU:HD12	2.12	0.50
1:A:265:SER:HB3	2:C:10:DT:H3	1.76	0.50
1:A:692:SER:HB2	1:A:842:THR:HG23	1.93	0.50
1:A:234:VAL:HA	1:A:251:ILE:O	2.12	0.49
1:B:279:GLU:HG3	1:B:281:HIS:HE1	1.77	0.49
1:B:696:MET:O	1:B:700:THR:HG23	2.11	0.49
1:A:183:THR:HG21	1:A:218:ILE:HD13	1.95	0.49
1:A:406:ILE:HD11	1:A:434:LYS:HE2	1.95	0.49
1:B:258:VAL:O	1:B:262:GLN:HG3	2.13	0.49
1:A:399:GLU:N	1:A:399:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:HG3	1:B:270:HIS:CE1	2.48	0.49
1:B:643:MET:CE	1:B:771:ILE:HA	2.43	0.49
1:B:778:ASN:HB3	1:B:827:TYR:CZ	2.48	0.49
1:A:272:LEU:HD11	1:A:275:LEU:HB2	1.94	0.48
1:A:493:GLU:HG2	1:A:536:GLN:CG	2.43	0.48
1:A:491:ILE:HD12	1:A:495:SER:HB3	1.96	0.48
1:A:281:HIS:HA	1:A:318:PHE:HZ	1.78	0.48
1:A:370:MET:N	1:A:371:LYS:HG2	2.28	0.48
1:B:119:LEU:HD23	1:B:248:ARG:CZ	2.44	0.48
1:B:194:ALA:HA	1:B:197:ARG:HH12	1.79	0.48
1:B:134:LEU:HD11	1:B:138:GLN:HE21	1.78	0.48
1:A:418:GLU:HG2	1:A:453:TRP:CZ2	2.49	0.47
1:B:387:TYR:HB2	1:B:392:LEU:HD21	1.96	0.47
1:B:850:ILE:HD13	1:B:867:LEU:HD23	1.96	0.47
1:A:509:ARG:HD3	1:A:526:GLU:OE1	2.14	0.47
1:A:428:PHE:O	1:A:507:SER:HB3	2.14	0.47
1:B:272:LEU:HD11	1:B:275:LEU:HB2	1.95	0.47
1:B:654:ASP:OD2	1:B:705:ARG:NH2	2.47	0.47
1:A:496:VAL:O	1:A:540:ARG:NH2	2.46	0.47
1:A:850:ILE:HG21	1:A:867:LEU:HD21	1.97	0.47
1:A:97:PHE:HD1	1:A:629:MET:HE3	1.79	0.47
1:A:99:HIS:HE2	1:A:111:GLU:CD	2.17	0.47
1:B:579:LEU:HG	1:B:632:ALA:HB2	1.96	0.47
1:A:236:TYR:HA	1:A:253:TYR:O	2.14	0.47
1:B:701:ILE:O	1:B:705:ARG:HG3	2.14	0.47
1:B:901:LEU:HD23	1:B:902:TYR:CE1	2.50	0.47
1:A:515:TYR:CE2	1:A:517:ILE:HD12	2.43	0.47
1:A:100:LEU:HD23	1:A:629:MET:HE2	1.97	0.47
1:A:678:ARG:NH1	4:A:1007:HOH:O	2.35	0.47
1:B:692:SER:HB2	1:B:842:THR:HG23	1.97	0.47
1:B:724:SER:O	1:B:728:GLN:HG2	2.15	0.47
1:A:690:MET:O	1:A:768:ARG:NH2	2.48	0.46
1:B:857:GLU:HG3	1:B:866:TYR:CE2	2.50	0.46
1:A:188:GLN:HE21	1:A:226:ARG:HH11	1.63	0.46
1:A:369:ARG:HB2	1:A:371:LYS:HE2	1.96	0.46
1:B:194:ALA:HA	1:B:197:ARG:NH1	2.31	0.46
1:B:78:ALA:HA	1:B:911:TYR:CD2	2.50	0.46
1:A:369:ARG:CB	1:A:371:LYS:HE2	2.45	0.46
1:A:734:LYS:HE3	1:A:734:LYS:HB2	1.79	0.46
1:A:190:LEU:HD21	1:A:307:ILE:CD1	2.46	0.46
1:B:333:VAL:HG12	1:B:334:MET:N	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:MET:HG2	1:A:373:GLU:HB2	1.97	0.46
1:A:406:ILE:HG22	1:A:441:ILE:HD12	1.98	0.45
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.77	0.45
1:B:182:LYS:HE2	1:B:309:MET:HB3	1.99	0.45
1:B:669:PHE:CZ	1:B:700:THR:HG21	2.51	0.45
1:B:846:PRO:HB3	1:B:875:PHE:CZ	2.52	0.45
1:B:644:ILE:CG2	1:B:741:LEU:HD11	2.47	0.45
1:B:467:GLN:HG3	1:B:471:GLN:HG3	1.98	0.45
1:B:765:PRO:HG2	1:B:927:GLU:HG2	1.98	0.45
1:B:145:LYS:NZ	1:B:149:ALA:HB2	2.32	0.45
1:B:215:ALA:CB	1:B:238:ILE:HD11	2.45	0.45
1:B:462:LEU:HD21	1:B:496:VAL:HG11	1.98	0.44
1:B:786:ARG:HD2	1:B:786:ARG:HH11	1.47	0.44
1:A:208:THR:HA	1:A:254:CYS:O	2.17	0.44
1:A:417:CYS:HB3	1:A:453:TRP:CZ3	2.52	0.44
1:B:461:PRO:HG3	1:B:673:LEU:HD12	1.99	0.44
1:B:232:ASN:O	1:B:246:ARG:HG2	2.18	0.44
1:A:778:ASN:HB3	1:A:827:TYR:CE2	2.53	0.44
1:B:129:ARG:O	1:B:133:GLU:HG3	2.18	0.44
1:B:670:TYR:CZ	1:B:723:SER:HB2	2.52	0.44
1:B:850:ILE:HG21	1:B:867:LEU:HD21	2.00	0.44
1:A:369:ARG:HB3	1:A:370:MET:H	1.48	0.44
1:B:346:LEU:HD13	1:B:394:LYS:HB2	1.99	0.44
1:B:429:LEU:HB3	1:B:430:PRO:HD2	2.00	0.44
1:B:104:ASN:OD1	1:B:105:PHE:N	2.49	0.43
1:B:767:LEU:O	1:B:771:ILE:HG12	2.17	0.43
1:B:147:LEU:HD23	1:B:147:LEU:O	2.18	0.43
1:B:67:ARG:NH2	1:B:71:LEU:HD21	2.33	0.43
1:B:333:VAL:HG12	1:B:334:MET:O	2.17	0.43
1:A:355:LYS:HG3	1:A:355:LYS:O	2.18	0.43
1:A:382:ARG:NH2	4:A:1017:HOH:O	2.52	0.43
1:A:643:MET:HG2	1:A:656:ILE:CG2	2.49	0.43
1:B:222:VAL:HG11	1:B:253:TYR:HE2	1.83	0.43
1:B:376:ILE:O	1:B:380:LEU:HG	2.18	0.43
1:A:351:TYR:CE2	1:A:408:PHE:HB2	2.54	0.43
1:B:91:ALA:HB2	1:B:902:TYR:HD2	1.83	0.43
1:B:476:ARG:HG2	1:B:477:ARG:N	2.34	0.43
1:B:798:MET:C	1:B:805:ARG:NH1	2.72	0.43
1:B:857:GLU:HG2	1:B:868:CYS:SG	2.59	0.42
1:A:346:LEU:HA	1:A:349:THR:HG22	2.00	0.42
1:A:417:CYS:HB3	1:A:453:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:VAL:HG12	1:A:836:LEU:HD23	2.01	0.42
1:B:764:ILE:HB	1:B:765:PRO:HD3	2.00	0.42
1:B:678:ARG:HH21	1:B:682:ILE:HD11	1.84	0.42
1:B:866:TYR:C	1:B:866:TYR:CD2	2.93	0.42
1:B:654:ASP:N	1:B:655:PRO:HD2	2.34	0.42
1:B:782:LEU:HD12	1:B:798:MET:HB2	2.02	0.42
1:A:281:HIS:HA	1:A:318:PHE:CZ	2.54	0.42
1:A:643:MET:HG2	1:A:656:ILE:HG23	2.01	0.42
1:B:642:LYS:O	1:B:646:MET:HG2	2.19	0.42
1:B:230:LEU:O	1:B:243:ARG:NH2	2.47	0.42
1:B:797:THR:HA	1:B:805:ARG:NH2	2.34	0.42
1:B:182:LYS:NZ	1:B:278:ASP:OD2	2.28	0.42
1:A:497:THR:HG22	1:A:543:ARG:NH1	2.35	0.41
1:A:899:LYS:HB3	1:A:899:LYS:HE3	1.87	0.41
1:B:390:ARG:O	1:B:394:LYS:HG3	2.20	0.41
1:B:66:GLU:O	1:B:70:GLU:HG2	2.19	0.41
1:A:778:ASN:O	1:A:826:VAL:HA	2.20	0.41
1:A:830:ARG:HE	1:A:836:LEU:HD21	1.83	0.41
1:A:888:LEU:HD21	1:A:919:ILE:HG12	2.02	0.41
1:B:647:SER:HB3	1:B:656:ILE:HG21	2.01	0.41
1:A:147:LEU:O	1:A:147:LEU:HD23	2.21	0.41
1:B:174:ILE:HD13	1:B:186:VAL:HG21	2.03	0.41
1:B:857:GLU:HG3	1:B:866:TYR:HE2	1.85	0.41
1:B:260:LEU:HD23	1:B:260:LEU:HA	1.94	0.41
1:A:207:CYS:O	1:A:253:TYR:HA	2.19	0.41
1:A:847:MET:O	1:A:851:ILE:HG13	2.21	0.41
1:B:134:LEU:HD11	1:B:138:GLN:NE2	2.34	0.41
1:A:379:TYR:CG	1:A:556:ALA:HB2	2.56	0.41
1:B:461:PRO:HB2	1:B:466:MET:CE	2.29	0.41
1:B:510:THR:CG2	1:B:511:LYS:N	2.84	0.41
1:A:174:ILE:HD13	1:A:186:VAL:HG21	2.02	0.41
1:A:807:ASN:O	1:A:837:PHE:HA	2.21	0.41
1:B:752:CYS:SG	4:B:1101:HOH:O	2.62	0.41
1:B:54:LEU:HD21	1:B:876:LYS:HG2	2.02	0.41
1:A:497:THR:HA	1:A:540:ARG:NH2	2.35	0.41
1:A:246:ARG:HH11	1:A:246:ARG:HD2	1.71	0.41
1:A:704:TYR:CZ	1:A:708:ARG:HD2	2.56	0.41
1:A:337:VAL:HG11	1:A:541:ALA:HB3	2.03	0.41
1:B:281:HIS:HA	1:B:318:PHE:HZ	1.85	0.41
1:B:158:TYR:CD1	1:B:330:ILE:HD12	2.56	0.41
1:B:530:THR:HG21	1:B:564:ILE:C	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:924:SER:O	1:B:927:GLU:HG3	2.21	0.41
1:A:373:GLU:HG2	1:A:377:GLU:CG	2.51	0.40
1:A:381:ARG:NH1	1:A:384:ARG:NH1	2.68	0.40
1:B:701:ILE:HG23	1:B:731:GLU:OE2	2.20	0.40
1:B:922:LEU:HA	1:B:922:LEU:HD23	1.90	0.40
1:B:655:PRO:HB3	1:B:698:HIS:CD2	2.56	0.40
1:B:652:CYS:HB2	1:B:767:LEU:CD2	2.51	0.40
1:B:901:LEU:HD23	1:B:902:TYR:CZ	2.51	0.40
1:A:277:LEU:HD21	1:A:290:LEU:HD13	2.02	0.40
1:A:430:PRO:HA	1:A:510:THR:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	841/944 (89%)	827 (98%)	14 (2%)	0	100	100
1	B	843/944 (89%)	822 (98%)	21 (2%)	0	100	100
All	All	1684/1888 (89%)	1649 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	757/842 (90%)	741 (98%)	16 (2%)	53 71
1	B	759/842 (90%)	740 (98%)	19 (2%)	47 67
All	All	1516/1684 (90%)	1481 (98%)	35 (2%)	50 69

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	94	GLN
1	A	114	GLU
1	A	115	ARG
1	A	243	ARG
1	A	272	LEU
1	A	355	LYS
1	A	369	ARG
1	A	671	SER
1	A	707	SER
1	A	711	HIS
1	A	714	ARG
1	A	734	LYS
1	A	830	ARG
1	A	867	LEU
1	A	928	ARG
1	B	102	SER
1	B	115	ARG
1	B	140	GLU
1	B	145	LYS
1	B	182	LYS
1	B	243	ARG
1	B	272	LEU
1	B	275	LEU
1	B	347	SER
1	B	452	ARG
1	B	485	VAL
1	B	540	ARG
1	B	686	MET
1	B	786	ARG
1	B	805	ARG
1	B	815	SER
1	B	818	SER
1	B	899	LYS
1	B	909	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	440	ASN
1	A	514	ASN
1	B	138	GLN
1	B	520	ASN
1	B	535	GLN
1	B	551	ASN
1	B	699	ASN
1	B	831	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	B	1001	1	4,4,4	0.77	0	6,6,6	0.69	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	634:LEU	C	635:PRO	N	1.20

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	849/944 (89%)	-0.17	2 (0%) 95 97	27, 48, 85, 122	0
1	B	851/944 (90%)	-0.13	4 (0%) 91 94	27, 47, 82, 147	0
2	C	9/9 (100%)	-0.03	0 100 100	53, 61, 80, 108	0
2	D	9/9 (100%)	-0.10	0 100 100	49, 60, 89, 109	0
All	All	1718/1906 (90%)	-0.15	6 (0%) 94 96	27, 48, 85, 147	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	ASN	3.2
1	A	518	GLU	2.6
1	B	681	GLU	2.5
1	B	786	ARG	2.3
1	B	795	ILE	2.3
1	A	53	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	B	1001	5/5	0.81	0.20	86,100,111,115	0

6.5 Other polymers (i)

There are no such residues in this entry.